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Reaction mechanism of the Li-driven electrochemical dehydrogenation of nanostructured complex hydrides

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Metal Hydrides (MH_x) have been proposed as potential candidates for negative electrode in Li-ion batteries [1]. Metal hydrides (MH_x) operate through the conversion reaction: $MH_x + xe^- + xLi^+ \rightleftharpoons M + xLiH$. They offer high capacity, suitable potential and low polarization. However, reaction kinetics and cycle-life need to be improved for practical applications. During the conversion reaction, the metal hydride suffers phase segregation into metallic species and LiH which needs to be restored during electrochemical cycling. Therefore, fast enough mass-transport of solid species has to be attained at room temperature which is only possible while using nanostructured hydrides.

The Li-driven electrochemical conversion reaction of nanocrystalline Mg_2MH_x complex hydrides (M=Fe, Co, Ni) has been investigated. These compounds accommodate transition metals to favor electronic conductivity within the electrode. The nanocrystalline compounds were synthesized by reactive ball milling [2]. From in situ X-Ray Diffraction (XRD) patterns collected during electrochemical discharge, an amorphization process has been identified [3]. The reaction mechanism has been analyzed in more detail by in situ X-ray absorption spectroscopy (XAS). The Li-driven decomposition reaction follows different reaction schemes for each transition metal M. For M = Fe, Co and Ni, the intermetallic sublattice separates into Fe+Mg, MgCo+Mg and Mg_2Ni, respectively, with different disorder effects depending whether there is segregation or not [4,5]. This sequence is in agreement with the corresponding binary M-Mg phase diagrams. According to these results, the electrochemical cycling properties of Mg_2MH_x (M=Fe, Co, Ni) compounds are expected to be highly dependent on the M metal.

Keywords: Li ion batteries, complex hydrides, conversion reaction, X-ray absorption spectroscopy